Scalable Dynamic Optimization

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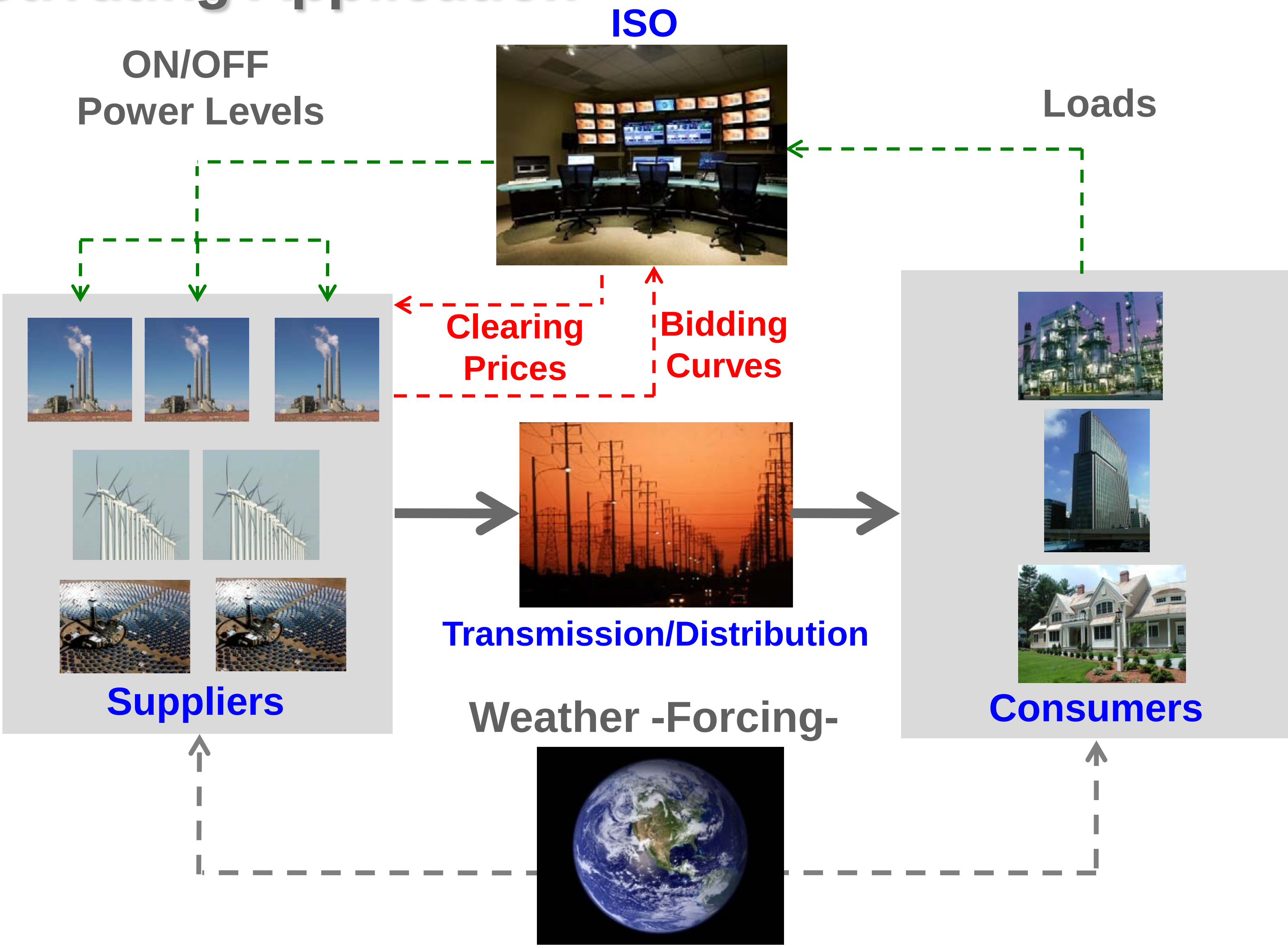
Motivating Application



Real-Time Optimization is Pervasive in Energy : Estimation, Management, Control

Requires Extreme-Scale NLP Solvers: Model Size and/or Short Time Scales

Technical Problem

Optimization Problem

$$\min_{x(t)} \frac{1}{2}(x(t)-\eta(t))^2 + \frac{1}{2}x(t)^2 \cdot \eta(t)$$

Steepest Descent

$$x^{j+1}(t) = x^j(t) - \nabla_x f(x^j(t), \eta(t))$$

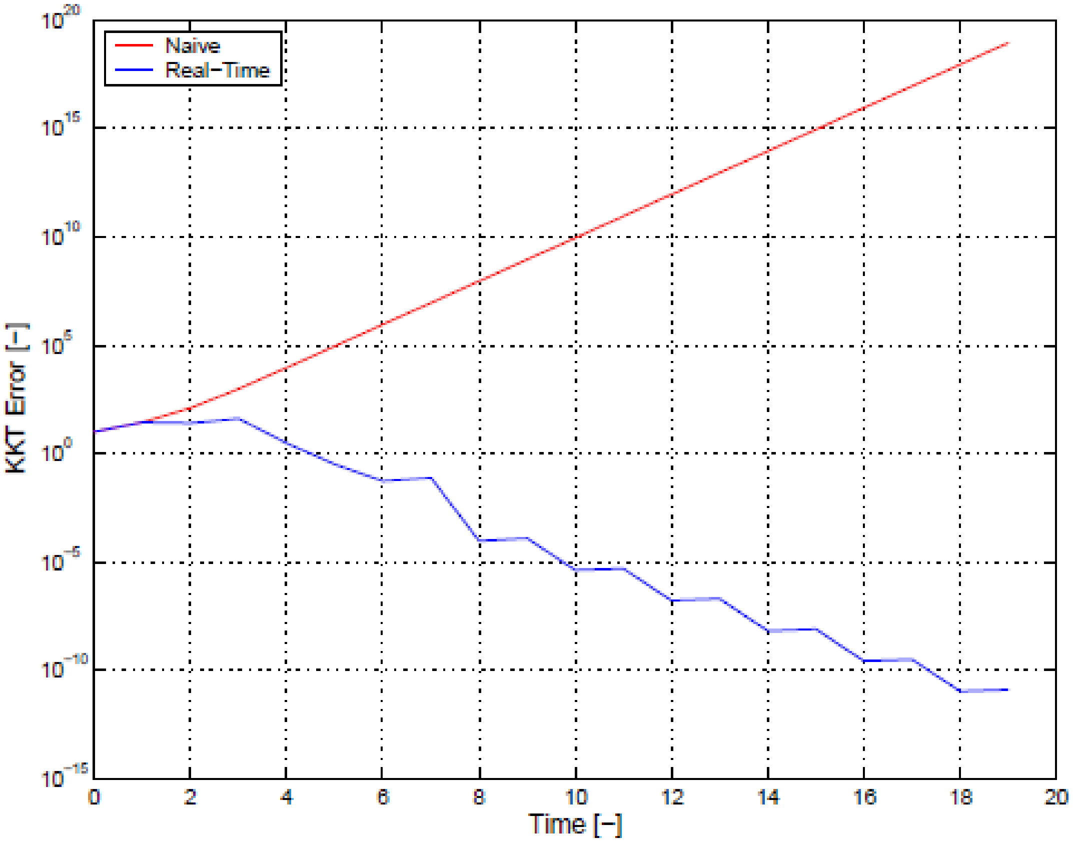
Iteration Latency

Dynamic System

$$\eta(t+(j+1)\cdot\Delta t) = \alpha \cdot \eta(t + j\cdot\Delta t)$$

Traditional : Solve to Given Accuracy (Neglect Dynamics)

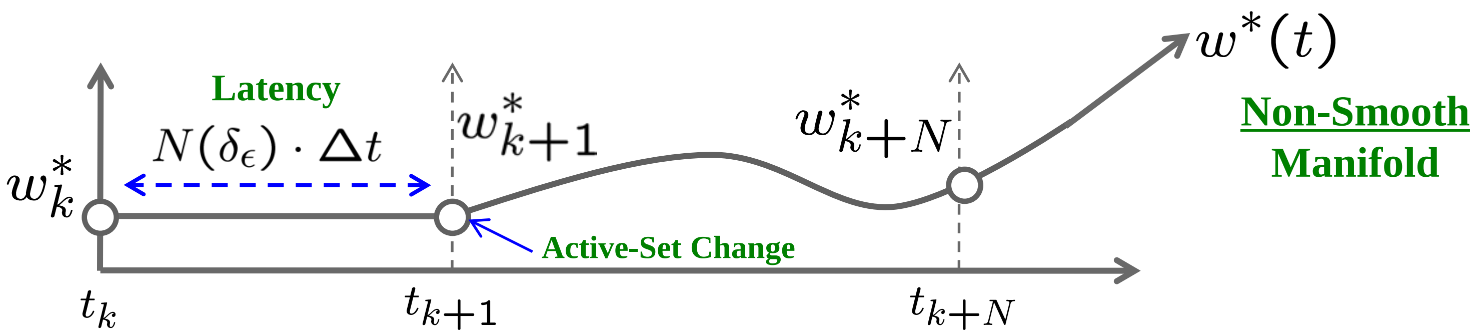
Real-Time : Interrupt at Sufficient Descent



Technical Problem

$$\begin{aligned} \min_{x}\ & f(x,t) \\ \text{s.t. } & h(x,t) = 0, \quad (\lambda) \\ & x \geq 0. \end{aligned} \qquad\qquad w^T = [x^T, \lambda^T]$$

Solution forms Time-Moving and Non-Smooth Manifold



- **Challenge is to Track Manifold Stably (Get Good Step with Minimum Latency)**

- **This requires NLP Solvers with the Following Features:**
    1) **Superlinear Convergence (Newton-Based)**
    2) **Scalable Step Computation (Enable Iterative Linear Algebra)**
    3) **Asymptotic Monotonicity of Minor Iterations (Makes Progress)**
    4) **Fast Active-Set Detection and Warm-Start**

- **Existing Solvers (Interior-Point and SQP) Fail at Least One Feature**

Exact Differentiable Penalty Functions (EDPFs)

Consider Transformation using Squared Slacks

$$\begin{aligned}\min_{x}\ & f(x) \\ \text{s.t. } h(x) &= 0 \\ x &\geq 0\end{aligned} \qquad\qquad \begin{aligned}\min_{x,z}\ & f(x) \\ \text{s.t. } h(x) &= 0 \\ x &= z^2\end{aligned}$$

Equivalent To:

$$\begin{aligned}\min_{z}\ & f(z^2) \\ \text{s.t. } h(z^2) &= 0\end{aligned} \qquad\qquad \mathcal{L}(z^2,\lambda) = f(z^2) + \lambda^T h(z^2)$$

$$\begin{aligned}\nabla_z \mathcal{L}(z^2,\lambda) &= 2 \cdot Z \cdot \left(\nabla f(z^2) + \nabla h(z^2)\lambda\right) \\ &= 2 \cdot X^{1/2} \nabla_x \mathcal{L}(x,\lambda)\end{aligned}$$

Apply DiPillo and Grippo's Penalty Function *DiPillo,Grippo, 1979, Bertsekas, 1982*

$$P(x,\lambda,\alpha,\beta) = \mathcal{L}(x,\lambda) + \frac{1}{2}\alpha c(x)^T c(x) + \boxed{2\beta \nabla_x \mathcal{L}(x,\lambda)^T X \nabla_x \mathcal{L}(x,\lambda)}$$

Solve NLP Indirectly Through EDPF Problem:

$$\min_{x,\lambda}\ P(x,\lambda,\alpha,\beta) \text{ s.t. } x \geq 0$$

EDPF

$$\begin{aligned} \min_x \ & f(x) \\ \text{s.t. } h(x) &= 0 \\ x &\geq 0 \end{aligned} \quad \longleftrightarrow \quad \min_{x,\lambda} \ P(x,\lambda,\alpha,\beta) \text{ s.t. } x \geq 0$$

$$P(x,\lambda,\alpha,\beta) = \mathcal{L}(x,\lambda) + \frac{1}{2}\alpha h(x)^T h(x) + 2\beta \nabla_x \mathcal{L}(x,\lambda)^T X \nabla_x \mathcal{L}(x,\lambda)$$

Advantages

- **EDPF Differentiable Everywhere**
- **Unconstrained Problem with Box Constraints**
- **Makes Progress at Each Iteration**

Questions

- **Under What Conditions Do Minimizers of EDPF and NLP Coincide?**
- **How to Deal with Nonconvexity?**
  - **Detect and Exploit Negative Curvature**
- **Can We Enable Scalability?**
  - **First and Second Derivatives**
  - **Iterative Linear Algebra**

Derivatives and Minimizers of EDPF

$$P(x,\lambda,\alpha,\beta) = \mathcal{L}(x,\lambda) + \frac{1}{2}\alpha h(x)^T h(x) + 2\beta \nabla_x \mathcal{L}(x,\lambda)^T X \nabla_x \mathcal{L}(x,\lambda)$$

In Compact Form

$$P_{\alpha,\beta}(w) = \mathcal{L}(w) + \frac{1}{2}\nabla_w \mathcal{L}(w)^T K_{\alpha,\beta}(w) \nabla_w \mathcal{L}(w) \qquad K_{\alpha,\beta}(w) = \begin{bmatrix} 4\beta X & \\ & \alpha I_m \end{bmatrix}$$

First Derivative

$$\nabla P = \nabla \mathcal{L} + \nabla^2 \mathcal{L} K \nabla \mathcal{L} + \frac{1}{2}\Gamma \mathrm{diag}(\nabla \mathcal{L}) \nabla \mathcal{L}$$

Is KKT Point of EDPF a KKT Point of NLP?

$$\begin{aligned} \sqrt{X}\nabla_x P &= 0 \\ \nabla_\lambda P &= 0 \end{aligned} \longrightarrow \begin{aligned} \sqrt{X}\nabla_x \mathcal{L}(x,\lambda) &= 0 \\ \nabla_\lambda \mathcal{L}(x,\lambda) &= 0 \end{aligned}$$

Theorem:

Under LICQ and SC there exist $\alpha, \beta,$ **such that KKT Point of EDPF is KKT point of NLP.**

Proof:

$$\begin{bmatrix} \mathbb{I}_{n\times n} + 4\beta\sqrt{X}\nabla_{x,x}\mathcal{L}(w^*)\sqrt{X} + 2\beta \mathrm{diag}\left(\nabla_x \mathcal{L}(w^*)\right) & \alpha\sqrt{X}\nabla_x h(x^*)^T \\ 4\beta \nabla_x h(x^*)\sqrt{X} & \mathbb{I}_{m\times m} \end{bmatrix} \begin{bmatrix} \sqrt{X}\nabla_x \mathcal{L}(w^*) \\ h(x^*) \end{bmatrix} = \begin{bmatrix} 0_n \\ 0_m \end{bmatrix}.$$

Matrix on LHS is PD For sufficient large α **and sufficiently small** β **.**

Note: Penalty parameters do not need to go to zero!

Derivatives and Minimizers of EDPF

Second Derivative

$$\nabla^2 P \cdot u = \nabla^2 \mathcal{L} \cdot u + \nabla^2 \mathcal{L} K \nabla^2 \mathcal{L} \cdot u + \nabla^2 \mathcal{L} \mathrm{diag}(\nabla \mathcal{L}) \Gamma \cdot u + \Gamma \mathrm{diag}(\nabla \mathcal{L}) \nabla^2 \mathcal{L} \cdot u + \nabla(\nabla^2 \mathcal{L} \cdot u) K \nabla \mathcal{L}$$

Third-Order Term

High-Order Term Vanishes at KKT Point Because $K \nabla \mathcal{L} = 0.$

Is Strict Minimizer of EDPF a Strict Minimizer of NLP?

Theorem:

i) **If KKT Point satisfies SSOC for NLP then there exist** $\alpha, \beta,$ **such that it satisfies SSOC of EDPF.**

ii) **If KKT Point does not satisfy SSOC for NLP then there exist** $\alpha, \beta,$ **such that this is not a strict local minimizer of EDPF.**

Proof: **Relies on Analysis of Projected Hessian where** N **is null-space matrix.**

$$\begin{aligned}
&\nu^T N^T \nabla^2 P N \nu \\
&= \begin{bmatrix} \nu_x^T N_x^T & \nu_\lambda^T \end{bmatrix} \begin{bmatrix} H & A^T \\ A & \end{bmatrix} \begin{bmatrix} N_x \nu_x \\ \nu_\lambda \end{bmatrix} \\
&\quad + \begin{bmatrix} \nu_x^T N_x^T & \nu_\lambda^T \end{bmatrix} \begin{bmatrix} H & A^T \\ A & \end{bmatrix} \begin{bmatrix} 4\beta X & 0 \\ 0 & \alpha \mathbb{I}_m \end{bmatrix} \begin{bmatrix} H & A^T \\ A & \end{bmatrix} \begin{bmatrix} N_x \nu_x \\ \nu_\lambda \end{bmatrix}.
\end{aligned}$$

Note: **Negative Curvature Strong Far From Solution!**

Derivatives and Minimizers of EDPF

A “Strong” Dennis-More Condition

Exact Hessian

$$\nabla^2 P \cdot u = \nabla^2 \mathcal{L} \cdot u + \nabla^2 \mathcal{L} K \nabla^2 \mathcal{L} \cdot u + \nabla^2 \mathcal{L} \mathsf{diag}(\nabla \mathcal{L}) \Gamma \cdot u + \Gamma \mathsf{diag}(\nabla \mathcal{L}) \nabla^2 \mathcal{L} \cdot u + \nabla(\nabla^2 \mathcal{L} \cdot u) K \nabla \mathcal{L}.$$

Approximate Hessian

$$Q \cdot u = \nabla^2 \mathcal{L} \cdot u + \nabla^2 \mathcal{L} K \nabla^2 \mathcal{L} \cdot u + \nabla^2 \mathcal{L} \mathsf{diag}(\nabla \mathcal{L}) \Gamma \cdot u + \Gamma \mathsf{diag}(\nabla \mathcal{L}) \nabla^2 \mathcal{L} \cdot u$$

Approximate Hessian is Asymptotically Convergent

$$\begin{aligned}(Q(w) - \nabla^2 P(w)) \cdot u &= \nabla(\nabla^2 \mathcal{L}(w) \cdot u) K(w) \nabla \mathcal{L}(w) \\ &= o(u) O(\|w - w^*\|), \quad \text{because} \quad K(w^*) \nabla \mathcal{L}(w^*) = 0 \\ &\overset{w \to w*}{=} 0.\end{aligned}$$

Implication:

- We Do NOT Need Third-Order Term to retain Superlinear Convergence
- However, Third-Order Derivatives Might Be Beneficial Early In Search

Trust-Region Newton

$$\min_{x,\lambda} \; P_{\alpha,\beta}(w) \text{ s.t. } w \in \Omega$$

- **Issue: Need to Detect and Exploit Directions of Negative Curvature**

- **Use Trust-Region Newton Framework of Lin and More (TRON)**

1) Determine Activity Using Cauchy Point

$$[w^c, \mathcal{A}^c] = \text{Proj}[w - \alpha^c \nabla P(w)]$$

2) Compute Search Step by Solving Trust-Region QP :
Steihaug's Preconditioned Conjugate Gradient Approach (PCG)

$$\begin{aligned}
\min_{\Delta w} \quad & \nabla P(w)^T \Delta w + \frac{1}{2} \Delta w^T Q(w) \Delta w \\
\text{s.t.} \quad & \Delta w_i = 0, \quad i \in \mathcal{A}^c \\
& \|\Delta w\| \leq \Delta
\end{aligned}$$

3) Check Progress Over Cauchy Step and Update Trust Region Radius

- **Approach Converges to Strict Local Minimizers of NLP Globally and Superlinearly**
- **Requires $\alpha, \beta,$ to Satisfy Conditions of Previous Theorems**

Computational Scalability

Derivatives

- EDPF Hessian Can be Assembled using Hessian and Jacobian Vector Products

$$\nabla^2 \mathcal{L} \cdot \nu = \begin{bmatrix} H & A^T \\ A & \end{bmatrix} \begin{bmatrix} \nu_x \\ \nu_\lambda \end{bmatrix} = \begin{bmatrix} H \cdot \nu_x + A^T \cdot \nu_\lambda \\ A \cdot \nu_x \end{bmatrix}.$$

Kernel

$$Q \cdot u = \nabla^2 \mathcal{L} \cdot u + \nabla^2 \mathcal{L} K \nabla^2 \mathcal{L} \cdot u + \nabla^2 \mathcal{L} \mathrm{diag}(\nabla \mathcal{L}) \Gamma \cdot u + \Gamma \mathrm{diag}(\nabla \mathcal{L}) \nabla^2 \mathcal{L} \cdot u$$

Requires 2 Unique Kernels

Conjugate Gradient

$$\min_{s_d^k} \; g^{kT} N^k s_d^k + \frac{1}{2} s_d^{kT} (N^k)^T Q^k N^k s_d^k$$
$$\text{s.t. } \|D^k N_j^k s_d^k\| \leq \Delta^k.$$

- Does Not Require Assembling Reduced Hessian
- Requires Action of Inverse Preconditioner $(D^k)^{-1} \cdot r$
- Incomplete Cholesky, PARDISO, Multigrid
- Negative Curvature Detected Externally (Not by Linear Solver)

Toy Problem – Algorithmic Behavior

$$
\begin{aligned}
\min \quad & (x_1 - 1)^2 + (x_2 - 2)^2 + (x_3 - 3)^2 + x_1 x_4 \\
\text{s.t.} \quad & x_1 x_4 + x_1 x_2 + x_3 = 4, \qquad (\lambda) \\
& x_1, x_2, x_3, x_4 \geq 0.
\end{aligned}
$$

					TR		**Min Eigenv.**		
k	P^k	g^k_{Proj}	ρ^k	$\Vert s^k\Vert$	$\Vert\Delta^k\Vert$	$\Vert Q^k - H^k\Vert$	$\underline{\lambda}(Q^k_d)$	$\underline{\lambda}(H^k_d)$	card$(\mathcal{A}^k_P)$
0	25.150	2.0e+2							0
1	3.449	5.9e+1	+3.26	2.5e−1	261.9	2.0e+2	-2.48	-22.67	0
2	3.449	5.9e+1	-0.70	0.0e+0	523.9	5.8e+1	-2.48	-22.67	0
3	3.449	5.9e+1	-0.62	0.0e+0	131.0	5.8e+1	-2.48	-22.67	0
4	3.449	5.9e+1	-0.33	0.0e+0	32.0	5.8e+1	-2.48	-22.67	0
5	3.449	5.9e+1	-0.28	0.0e+0	8.0	5.8e+1	-2.48	-22.67	0
6	1.533	2.5e+1	+0.37	2.0e+0	2.0	5.8e+1	-2.48	-22.67	0
7	0.945	1.6e+0	+0.52	1.9e−1	2.0	2.9e+1	+0.15	-0.39	0
8	0.944	4.9e−1	+0.48	2.6e−3	4.0	1.9e+0	+0.19	+0.37	0
9	0.943	4.5e−1	+0.93	1.4e−3	4.0	4.0e−1	+0.19	+0.25	0
10	0.909	2.3e−1	+0.94	1.8e−1	8.0	3.4e−1	+0.40	+0.40	1
11	0.908	1.7e−6	+0.99	8.7e−3	16.0	3.1e−6	+0.38	+0.38	1

- **Trust Region Management Critical**
- **Line Search Solvers Fail (Range of Penalty Parameters Narrower)**

Predictive Control

$$\min \int_0^T \left(\alpha_c \cdot (c(\tau) - \bar{c})^2 + \alpha_t \cdot (t(\tau) - \bar{t})^2 + \alpha_u \cdot (u(t) - \bar{u})^2\right) d\tau$$

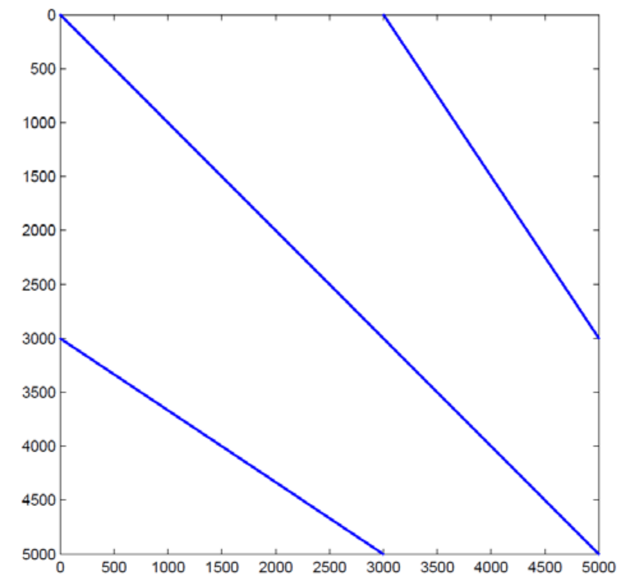
$$\text{s.t.} \quad \dot{c}(\tau) = \frac{1 - c(\tau)}{\theta} - p_k \cdot \exp\left(-\frac{p_E}{t(\tau)}\right) \cdot c(t)$$

$$\dot{t}(\tau) = \frac{t_f - t(\tau)}{\theta} + p_k \cdot \exp\left(-\frac{p_E}{t(\tau)}\right) \cdot c(\tau) - p_\alpha \cdot u(\tau) \cdot (t(\tau) - t_c)$$

$$c(\tau), t(\tau), u(\tau) \geq 0, \qquad \tau \in [0, T]$$

$$c(0) = c(\tau_{sys}), \qquad t(0) = t(\tau_{sys}).$$

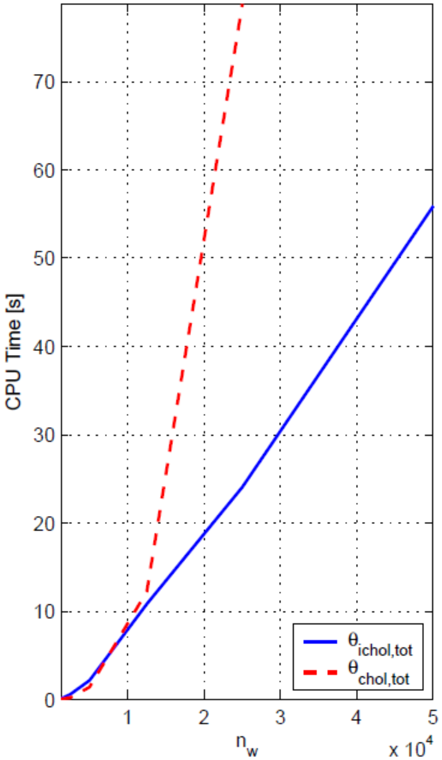
N	n	m	n_w	nnz($\nabla^2\mathcal{L}$)	nnz(Q)	%dens($\nabla^2\mathcal{L}$)	%dens(Q)
500	1,500	1,000	2,500	10,486	26,492	2.0e−1	4.0e−1
1,000	3,000	2,000	5,000	20,996	52,972	8.4e−2	2.0e−1
5,000	15,000	10,000	25,000	104,996	264,972	1.6e−2	4.0e−2
10,000	30,000	20,000	50,000	209,996	529,972	8.3e−3	2.1e−2

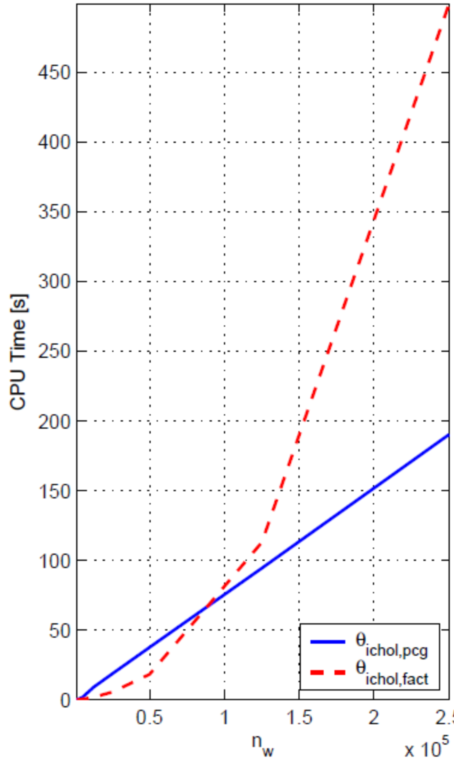


- Discretize and Scale Problem Up by Increasing Horizon N
- Sparsity of Augmented System Retained in Hessian of EDPF
- Drop Tolerance Incomplete Cholesky of 1e-4

Predictive Control - Scalability

		Incomplete Cholesky			Full Cholesky		
n_w	it_{pcg}	$\theta_{ichol,pcg}$	$\theta_{ichol,fact}$	$\theta_{ichol,tot}$	$\theta_{chol,pcg}$	$\theta_{chol,fact}$	$\theta_{chol,tot}$
1,250	17	8.5e−2	3.1e−2	1.1e−1	2.7e−2	3.3e−2	6.0e−2
2,500	24	4.9e−1	1.3e−1	6.2e−1	1.1e−1	1.5e−1	2.6e−1
5,000	29	1.7e+0	4.4e−1	2.2e+0	5.7e−1	8.5e−1	1.4e+0
12,500	31	9.0e+0	1.8e+0	1.1e+1	3.8e+0	8.4e+0	1.2e+1
25,000	31	1.8e+1	5.5e+0	2.4e+1	2.5e+1	5.4e+1	7.8e+1
50,000	31	3.7e+1	1.8e+1	5.5e+1	-	-	-
125,000	31	9.4e+1	1.1e+2	2.0e+2	-	-	-
250,000	31	1.9e+2	4.9e+2	6.8e+2	-	-	-





- Scalability of Full Cholesky Not Competitive
- Incomplete Cholesky Gives High Flexibility
  Can Specify Drop Tolerance to Reduce Latency
- PCG Iterations Scale Well
- Largest Problem : 250,000 Variables

Predictive Control – Active Sets

	Case 1				Case 2			
k	P^k	g^k_{Proj}	$\mathcal{A}_P(w^k)$	n^k_{PCG}	P^k	g^k_{Proj}	$\mathcal{A}_P(w^k)$	n_{PCG}
0	4.05e+3	4.52e+3	44	-	1.21e+4	2.43e+5	173	-
1	1.14e+2	4.70e+3	44	41	4.96e+2	5.76e+4	0	132
2	1.83e+1	3.72e+3	119	32	9.48e+1	1.86e+3	0	45
3	1.83e+1	1.55e+2	170	27	5.57e+0	3.27e+4	26	37
4	1.83e+1	5.59e−6	173	17	3.98e+0	1.11e+3	43	26
5	-	-	-		3.98e+0	8.50e−6	44	13

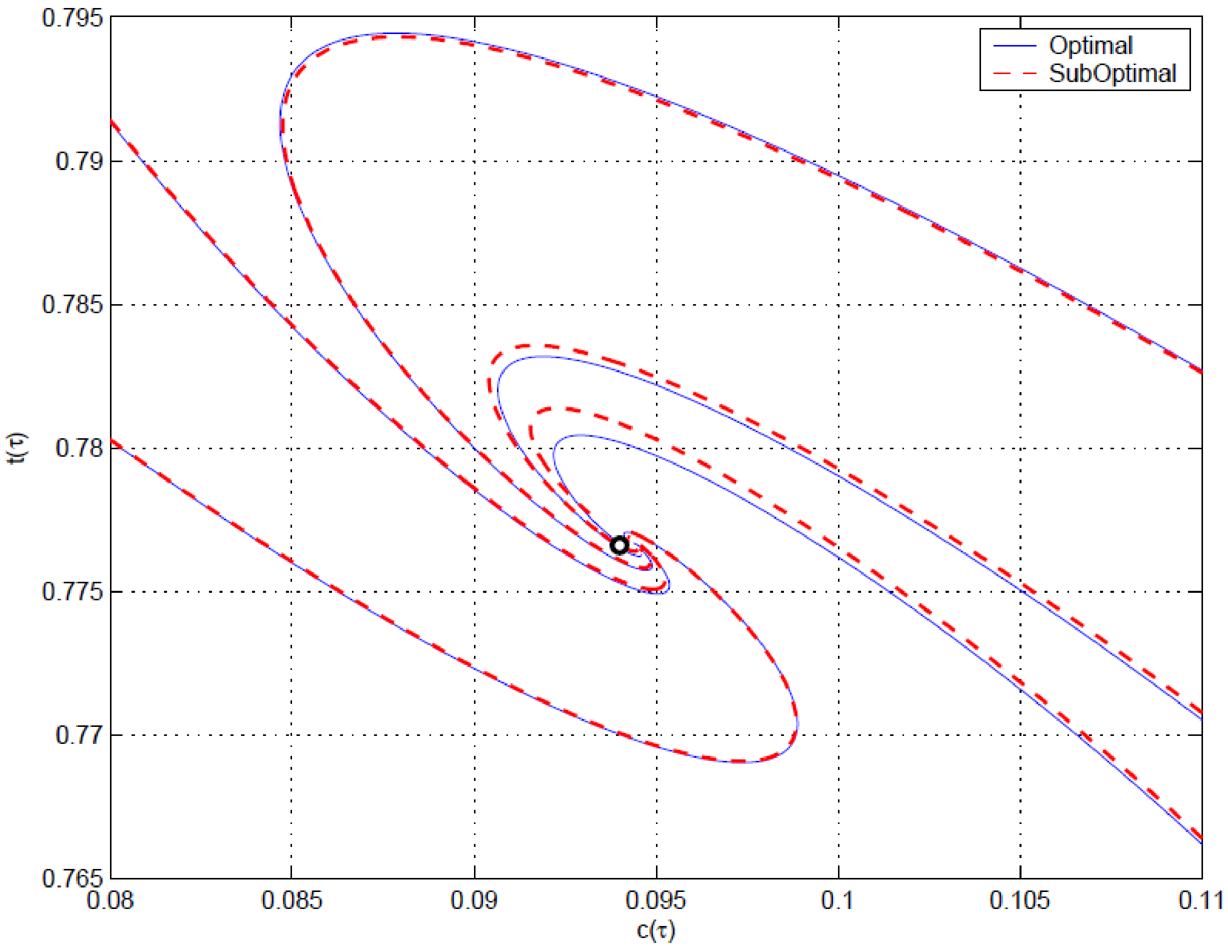
- Case 1) 173 variables active at solution and initialized at point with 44

- Case 2) 44 variables active at solution and initialized at point with 173

- Cauchy Search Efficient at Detecting Activity (Allows for Large Changes Between Iterates)

- Number of PCG Iterations Do Not Degrade as Solution Approaches (Compare with IP)

Predictive Control – Early Termination



- Run Problem Terminating After 2 Major Iterations and 20 PCG iterations

- Reduced Latency by A Factor of 4 (Four)

- Convergence to Equilibrium Point (Warm-Starting Effective)

Conclusions and Future Work

- **It is possible to derive NLP algorithms with?**

  1) **Superlinear Convergence (Newton-Based)**
  2) **Scalable Step Computation (Enable Iterative Linear Algebra)**
  3) **Asymptotic Monotonicity of Minor Iterations (Makes Progress)**
  4) **Active-Set Detection and Warm-Start**

- **Critical in “Fast” Real-Time Environments**

- **Proposed Approach : EDPF + Trust-Region Newton + PCG**
  1) **Newton-Based in Primal/Dual Space with Convergent Approximate Hessian**
  2) **Steihaug’s PCG to Detect and Exploit Negative Curvature**
  3) **PCG Improvement on EDPF Function**
  4) **Cauchy**

- **ToDo:**
  - **Connections with Other Penalty Methods (Augmented Lagrangians)**
  - **More Robust Implementation (Scaling, Trust-Region Update Rules, Ill-Conditioning)**
  - **Alternative Penalty Functions Requiring Only One Parameter**
  - **Preconditioning**
  - **Exploiting Special Structures**